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Armstrongite from Khan Bogdo (Mongolia): Crystal structure determination and implications for zeolite-like cation exchange properties

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Abstract

The results of a combined electron probe microanalysis, single-crystal X-ray diffraction, and Fourier transform infrared study of a crystal of armstrongite from Khan Bogdo deposit (Gobi, Mongolia) are reported. Major element analysis provided (wt%): CaO 9.2(1), ZrO_2 20.9(2), and SiO_2 62.5(2). Significant concentrations of REE (0.45 wt%) were also detected. From single-crystal structural refinement, armstrongite resulted monoclinic [space group *C*2/*m*, *a* = 14.0178(7), *b* = 14.1289(6), *c* = 7.8366(3) Å, β = 109.436(3)°, *V* = 1463.6(1) Å^3, *Z* = 4] and twinned with two individuals rotated around a twin twofold axis parallel to [100]. The analyzed crystal was refined up to *R* = 3.3% (R_w = 2.9%). The structural refinement showed that the investigated armstrongite has only two water groups per formula unit consistent with the infrared analysis. Indeed, the occurrence in the infrared spectrum of the armstrongite (here reported for the first time) of two bending vibration bands at about 1640 and 1610 cm^{-1} testifies to the presence of two water groups environments. The results of this integrated approach converged to the following empirical formula (based on Si = 6 atoms per formula unit): $(Ca_{0.96}Ce_{0.01}Yb_{0.01})Zr_{0.99}Si_6O_{14.97}\cdot 2.02H_2O$. Finally, the studied mineral shows a framework density (FD = 21.86) lying in the range of zeolites and microporous heterosilicates with tetrahedral-octahedral frameworks. The determined crystal chemical features are relevant for the possible employment of this mineral or of its synthetic analogs for technological applications.

Keywords: Armstrongite, microporous Zr-silicates, single-crystal structure refinement, EPMA, infrared analysis, water groups